



# Science for Environment Policy

## New research suggests that alternatives to legacy PFASs may be no safer

**PFASs — per- and polyfluoroalkyl substances — are a family of chemicals used in a wide range of industrial and consumer applications.** Due to concerns about their persistence, bioaccumulation and toxicity, long-chain PFASs are increasingly being phased out, creating a growing market for alternatives. Researchers have developed a novel method, based on molecular simulation techniques, to estimate the rate at which novel PFASs interact and bind with particular proteins ('binding affinity') — an important factor in determining a substance's bioaccumulation potential in organisms. The method indicates that replacement PFASs may be just as bioaccumulative as original (legacy) PFASs and are, therefore, not necessarily safer. If correct, this finding has significant policy implications.

**It is estimated that there are more than 4 000 PFASs on the global market; these chemicals are often used in products such as fire-fighting foams, food contact materials, and clothing.** Concerns have been raised about the persistence, bioaccumulation and toxicity of long-chain PFASs. This has led to the phasing out of their production for the majority of uses and the increasing use of replacement PFASs, such as perfluoroether carboxylic acids (PFECAs) and perfluoroether sulfonic acids (PFESAs). However, information on the identity, frequency of use, and potential impacts of these alternative PFASs remains scarce.

A rapid and reliable method to predict how these chemicals behave in the environment and within organisms would be of significant benefit in hazard and risk assessment. A novel *in-silico* (computer simulated) method based on molecular dynamics has been proposed to predict PFAS-protein interactions — the method is suitable for large-scale screening. The researchers intend this method to give insight into how PFASs accumulate within organisms, and to provide information and parameters for use in physiologically-based pharmacokinetic (PBPK) models, which are used to predict how drugs and other chemical substances are absorbed, distributed, and excreted in the body.

As a test, the method was used to estimate the relative binding affinity of a total of 15 legacy and replacement PFASs for human and rat liver-type fatty acid binding proteins (hLFABP and rLFABP). The results were compared to experimental data extracted from three pre-existing studies. Overall, there was good correlation between the simulated and measured binding affinities, with correlation coefficients of 0.97, 0.79, and 0.96.

In total, five replacement PFASs were assessed: three PFECAs (ADONA, GenX, and EEA) and two PFESAs (F-53 and F-53B). The results suggest that EEA and ADONA are at least as strongly bound to rLFABP as the legacy PFAS perfluoroheptanoic acid (PFHpA) and as strongly bound to hLFABP as the legacy PFAS perfluorooctanoic acid (PFOA). Both F-53 and F-53B had similar or stronger binding affinities than the legacy PFAS perfluorooctanesulfonate (PFOS). Since protein-PFAS interactions are important determinants of bioaccumulation potential in organisms, these findings indicate that these alternatives are not necessarily safer than long-chain legacy PFASs.

From a policy perspective, these findings are likely to influence new substance groups considered by the European Human Biomonitoring Initiative (HBM4EU). Moreover, this research has implications for hazard and risk assessment of non-tested PFASs, as it provides a novel method for the large-scale screening of protein-PFAS interactions. Such screening is economically and logistically desirable, especially given the potentially vast number of PFASs on the market and the limited resources available for their evaluation.

**22 November 2018  
Issue 517**

**Subscribe to free  
weekly News Alert**

**Source:** Cheng, W. and Ng, C. A. (2018). Predicting Relative Protein Affinity of Novel Per- and Polyfluoroalkyl Substances (PFASs) by An Efficient Molecular Dynamics Approach. *Environmental Science & Technology*, 52: 7972-7980. DOI: 10.1021/acs.est.8b01268.

**Contact:**  
[carla.ng@pitt.edu](mailto:carla.ng@pitt.edu)

**Read more about:**  
[Chemicals](#), [Emerging risks](#), [Innovation and new technologies](#), [Risk assessment](#)

The contents and views included in Science for Environment Policy are based on independent, peer-reviewed research and do not necessarily reflect the position of the European Commission. Please note that this article is a summary of only one study. Other studies may come to other conclusions.

To cite this article/service: "[Science for Environment Policy](#)"; European Commission DG Environment News Alert Service, edited by SCU, The University of the West of England, Bristol.